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| Title: | LANL Accelerator Activities for C-band |
| Author(s): | Krawczyk, Frank L. |
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# LANL Accelerator Activities for C-band

**Frank Krawczyk**

**AOT - Accelerators and Electrodynamics**

**LANL**

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# Abstract


- LANL has a range of accelerator activities that would benefit from improvements in RF resonator performance. XFEL (presently using a SRF baseline similar to LCLS-II) would benefit from much higher gradient and long-pulse operation of copper structures. Higher gradient RF structures for lower energy accelerators (~100 MeV) would also provide a path to transportable systems, such as ICS sources. Lastly, the utilization of dielectrics could be exploited for increased efficiency and compactness, e.g. for accelerator in space efforts. A LANL R&D effort aims at systematic improvement of copper structures employing material science simulations to explain and improve breakdown effects, combined with highly optimized designs, integration of cryo-cooling and the use of dielectric insertions. The work is integrated into a High-Gradient collaboration between SLAC, UCLA and LANL.

# LANL Accelerator Activities for C-band

2/14/2019

SLAC Accelerator Seminar

Los Alamos
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- LANL Accelerator Projects
  - Overview
- Technology limitations
  - Gradient, pulse length, burst mode
- Start-up R&D effort
  - Choice of Frequency
  - Material Science tools
  - Dielectric insertions
- Full Technology R&D effort
- Summary and Outlook

# LANL Accelerator Efforts – An Overview

New accelerator projects starting at LANL since 2018

- SCORPIUS, a multi-pulse induction linac for hydrodynamic experiments
- DMMSC (Dynamic Mesoscale Materials Science Capability) with a trajectory leading to a MaRIE type XFEL
- Accelerator in Space (AIS) in support of the NASA CONNEX mission. The goal is to study magnetospheric processes and their role for different types of auroral and ionospheric activities
- Compact accelerators for national defense missions, e.g transportable accelerator driven ICS sources
- Build-up of an Accelerator Development and Engineering Facility (ADEF), a local electron beam based test facility for technology development
- Neutral Particle Beam technology development for the DoD

# Technology limitations (selective list)

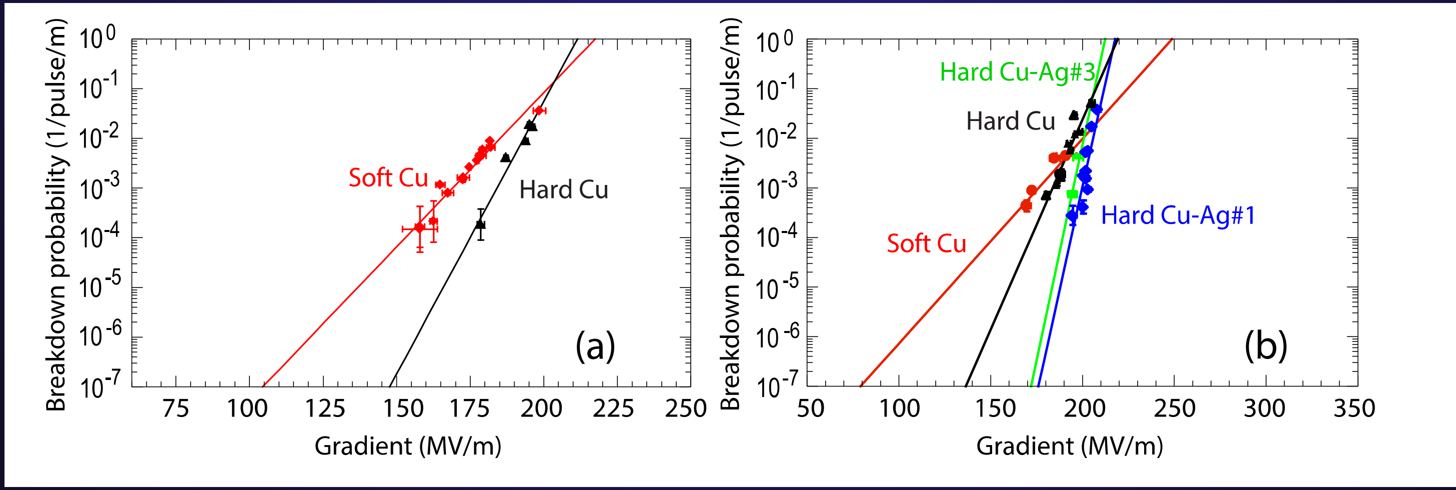
- Size, cost and operation needs of facility size systems like MaRIE
  - The location at LANSCE imposes a length limit on the linac
  - SRF option (LCLS-II like) has no energy upgrade path
  - SRF option enables long-pulse operation, but low frequency limits pulse formats
  - High frequency normal conducting RF (NCRF) has potential for much higher gradient, but is limited in pulse length and has high RF-losses
- Size, weight and power efficiency (SWaP) of space application accelerator
  - SRF systems are large and have complex sub-systems
  - High-frequency resonators are small, but NCRF is still heavy and has high RF-losses
- Size of compact, transportable accelerator systems
  - Transport requirement (container size) limits accelerator length

# Start-up R&D effort

- FY19 Feasibility Study with the following thrust areas
  - **Address breakdown limitations to achieve ultra high gradients (UHG) in copper structures (development and verification of tools)**

# Material Simulation Effort

- Incidence of breakdown is very well characterized (SLAC, CERN, KEK, INFN-LNF, etc.)
- Microscopic causes are complex:
  - occurs at fields that are well below what needed of a clean flat Cu surface (~10 GV/m)
  - requires the formation of precursors that locally enhance the field
  - How does precursor formation couple with the microstructure and composition?




Simakov, Dolgashev, Tantawi, 2018

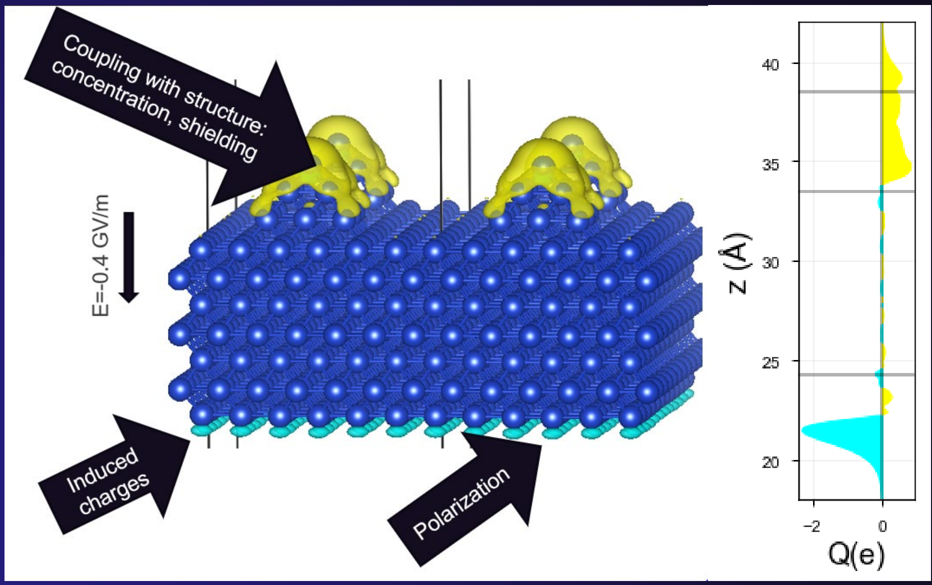
# Modeling Goals

- **Short-term goals:**
  - **Demonstrate that the response of metals to external E fields can be captured by a classical approach calibrated by quantum calculations**
  - **Demonstrate a long-time and a large-scale atomistic simulations capability for metals under strong E fields**

- Long(er)-term goals:
  - Include combined H,E effects
  - Understand how the breakdown propensity of these defects couple to the microstructure and composition of the material
  - Inform the design of optimized material solutions

# Quantum Approach – Density Function Theory (DFT)

- Quantum description:
  - Explicit description of the electron gas
  - Variational approach: find the electronic density that minimizes quantum Hamiltonian
- Strengths:
  - Very accurate (~100 meV/atom)
  - First principles (few parameters, transferable)
- Weakness:
  - Very expensive (scales as $N_{electrons}^3$)
    - Small systems (~few 100 atoms): cannot capture microstructure effects
    - Static or short dynamic simulations (~ps): cannot explicitly simulate surface evolution




Example from VASP

- Determines equilibrium charge distribution
- Change in work-function to release charges

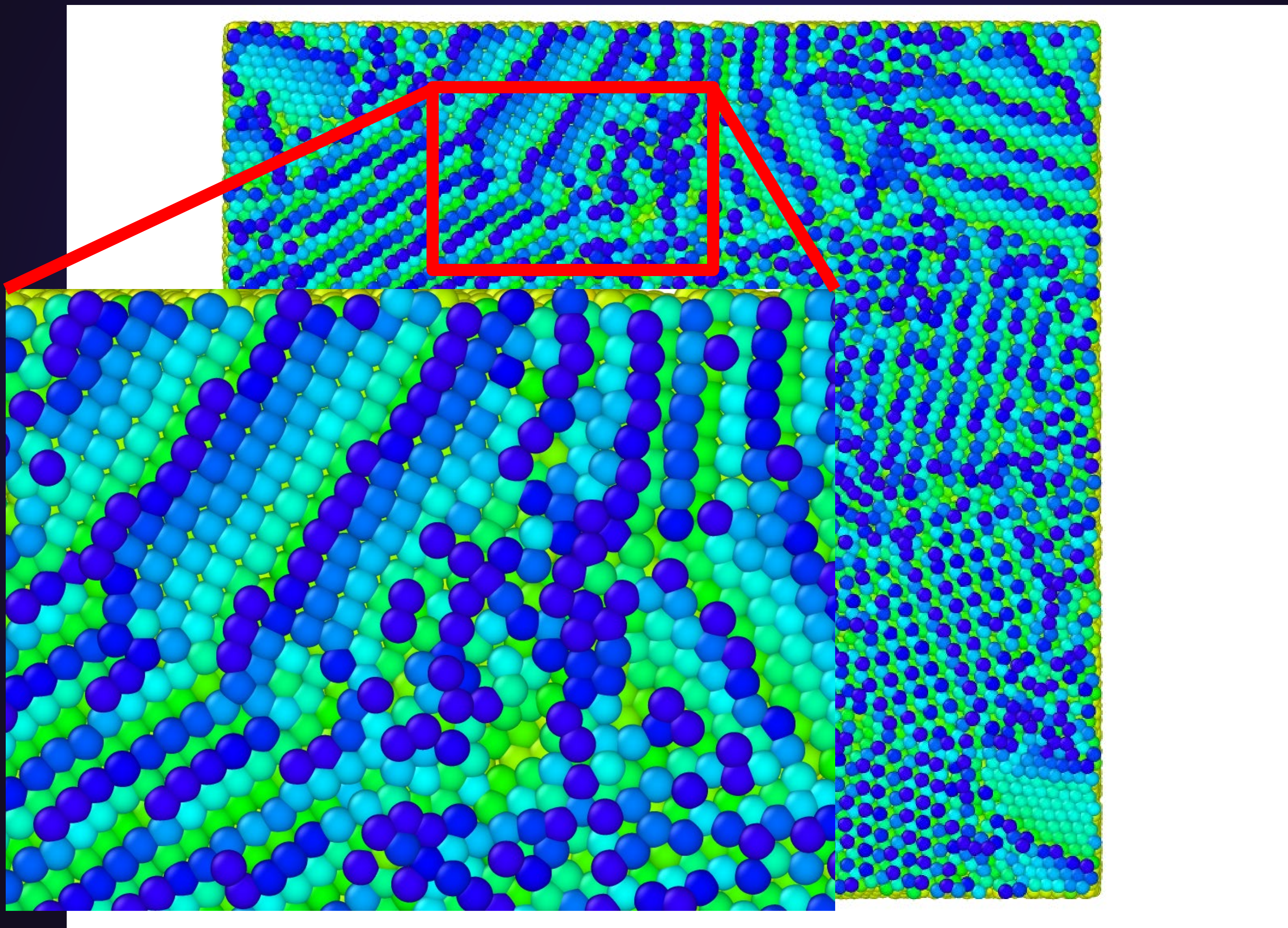
**Why are we doing this?**

**Fit classical model on DFT data – is well established process for copper**

# Classical Approach – Molecular Dynamics (MD)

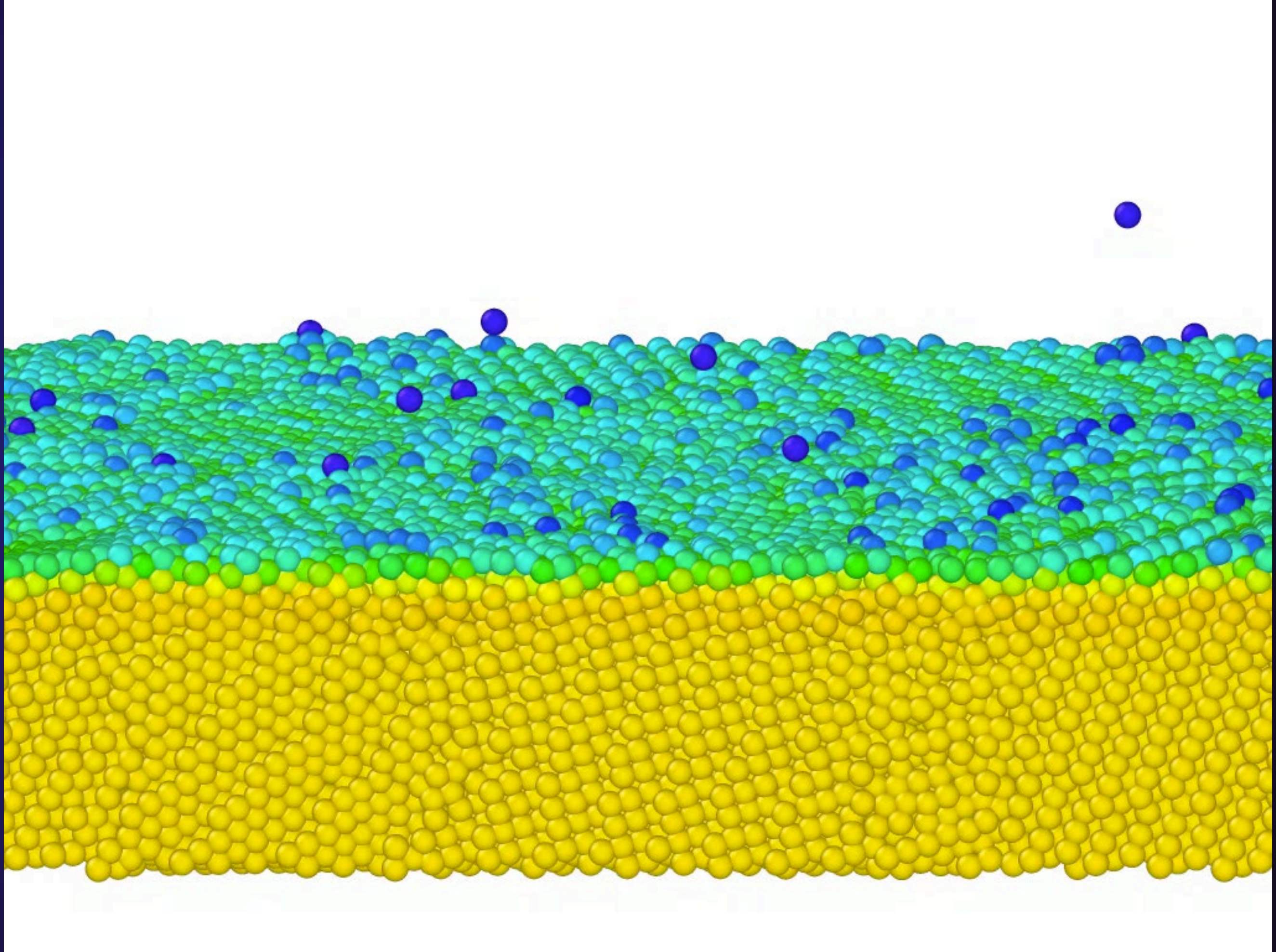
- Classical description:
  - Molecular dynamics (integration of classical EOM)
  - Charge-equilibration formalism (qEq) to capture effect of induced charges
- Strengths:
  - Reasonably accurate empirical description of Cu
  - Relatively fast
    - “Large” systems (~$10^6$ atoms): can capture some microstructural effects
    - “Long” simulations (milliseconds): can capture surface evolution
- Weakness:
  - Scales are still very limited compared to engineering scales

# LAMPPS modeling of charge equilibrated surface

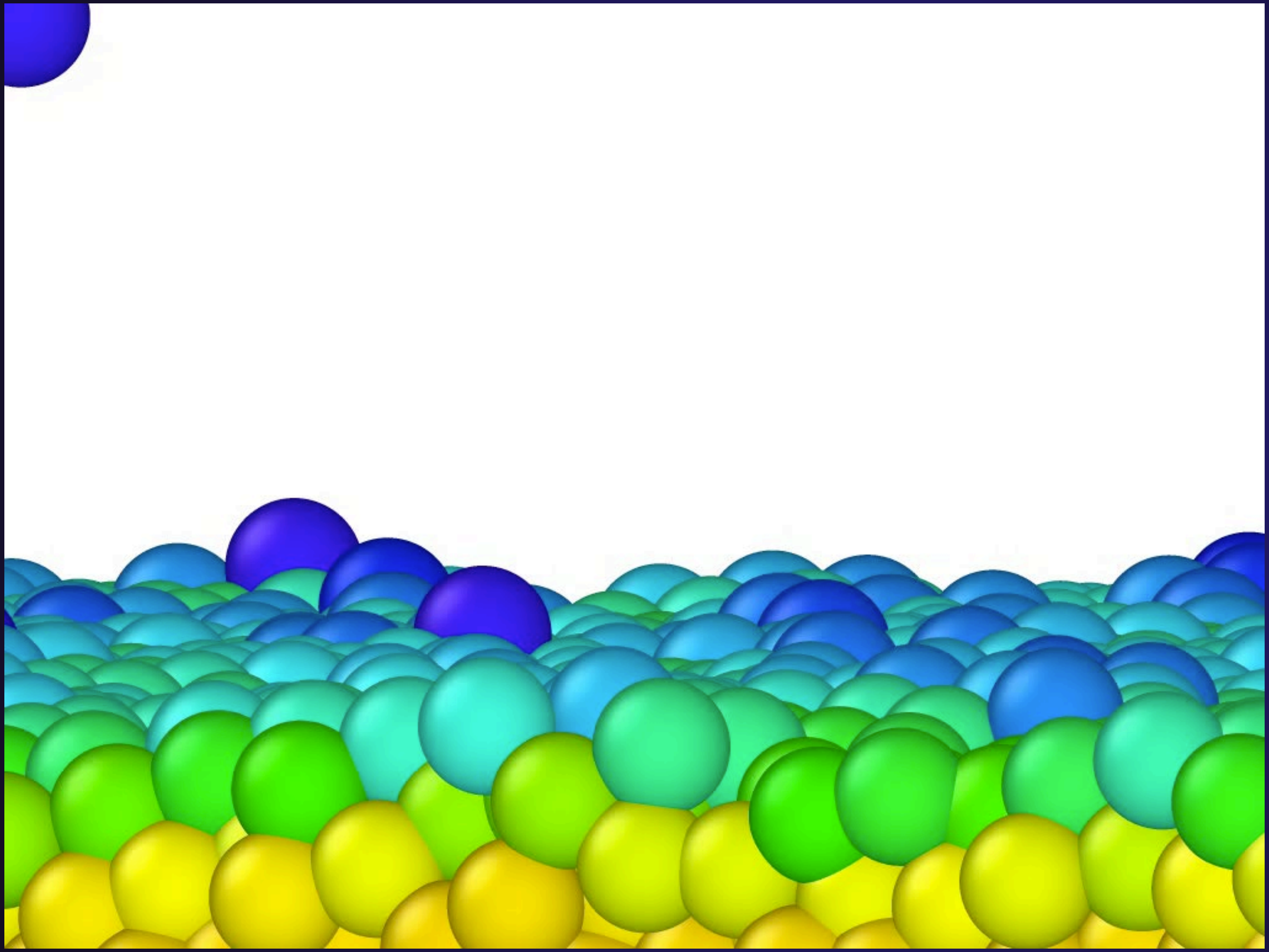


# MD under (very) strong field

- ~100,000 atoms
- polycrystalline sample
- 20x20 nm slab
- T=800K
- E=~10 GV/m (close to critical DC field)



# MD under (very) strong field



- Nano-pyramids spontaneously form, leading to local field enhancement and evaporation/field emission
- Suggests that breakdown can be simulated in very high-field configurations
- Can this mechanism create breakdown precursors?

# Future MD work: nature of the precursors

- Clear indications that magnetic fields are crucial
- Pulse heating is known to be a factor
- Will explore microstructural changes induced by thermal fatigue and their coupling with E and with the microstructure
- We have extended LAMPPS for consideration of harmonic E and H external forces

# State of the Material Simulation Work

- Classical models parameterized from quantum calculations can describe the energetics of metals under high fields
- In critical conditions, we see the spontaneous formation of nano-pyramids and the emission of atoms (i.e., “breakdown”)
- Still have to simulate the growth of the precursors
- Atomistic simulations face a serious challenge of scales, but can provide unique insights

# Start-up R&D effort

LANL pursues as small set of technology developments to address this range of performance issues

- FY19 Feasibility Study with the following thrust areas
  - Address breakdown limitations to achieve ultra high gradients (UHG) in copper structures (development and verification of tools)
  - **Identify best operation frequency for LANL-XFEL type applications**

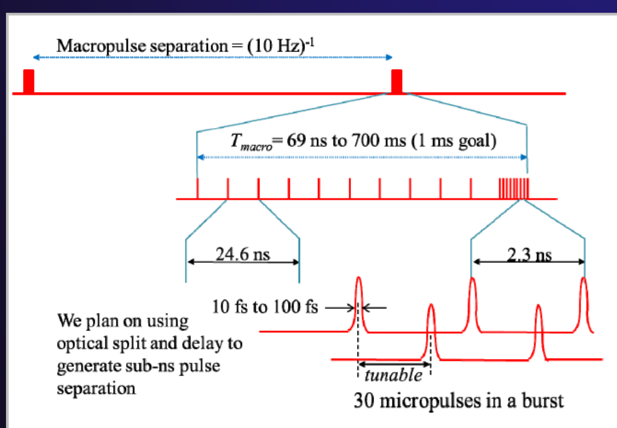
# LANL-XFEL needs (Expect the answer to be C-band)

- Space limitations

12 GeV @ 31.5 MV/m
➔ linac length ~750m


12 GeV @ 100 MV/m
➔ linac length ~170m

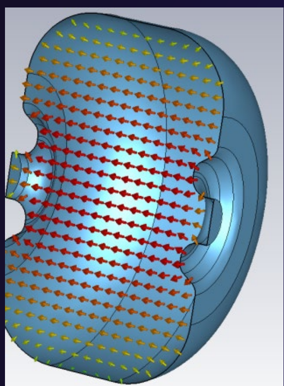
- Burst mode




S-band: slow, bunch spacing too close
X-band: beam quality limited by wakes
C-band: considered overall good mix

# Quantitative Comparison of L-, S-, C- and X-band

- RF properties (identical geometry, scaled S→C→X, a/λ 0.05 radius)

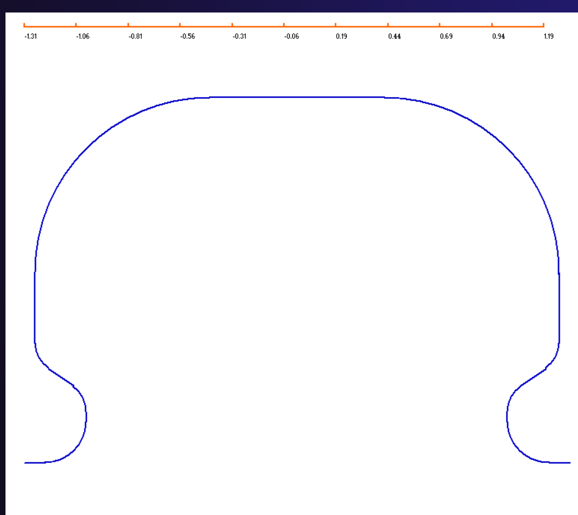


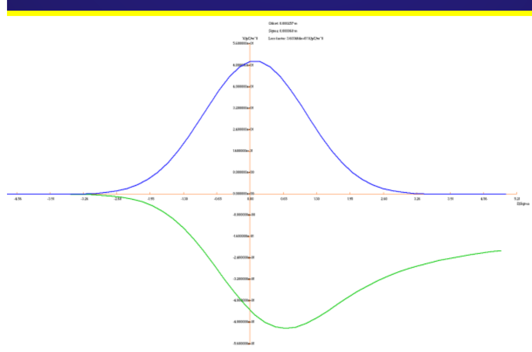
| | unit | S | C | X |
|---|---|---|---|---|
| **Frequency** | GHz | 2.856 | 5.712 | 11.424 |
| **Q0 (@ RT)** | | 1.90E+4 | 1.34E+4 | 9.48E+3 |
| **R/Q** | Ohm | 235.86 | 235.86 | 235.86 |
| **Ep/E0T** | | 2.9762 | 2.9762 | 2.9762 |
| **Hp/E0T** | mA/MV | 2.736 | 2.736 | 2.736 |
| **R Shunt** | MOhm/m | **85.162** | **120.437** | **170.323** |

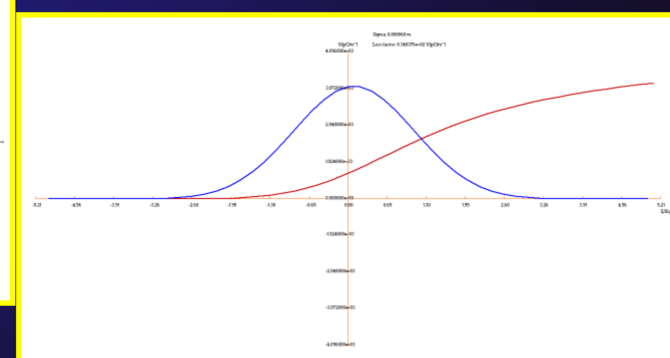
*Table 1: Critical performance among frequencies*

| (bold is better) | L-band | S-band | C-band | X-band |
|---|---|---|---|---|
| $R_{Shunt}$ [MΩ/m] | **9e6** | 85 | **120** | **170** |
| $k_{loss}$ long. [V/pC] | **10.2** | **26.4** | **36.4** | 50.4 |
| $k_{loss}$ trans. | **15.1** | **155** | **835** | 4420 |
| Gradient [MV/m] | 30 | 50 | **100** | **150** |
| Bunch sep. in burst | 3 cyc. | 6 cyc. | **13 cyc.** | **26 cyc.** |

- Short-range Wakes





Longitudinal and transverse wakes with ECHO

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  - **Integrate NCRF-design concepts with cryogenic operation**

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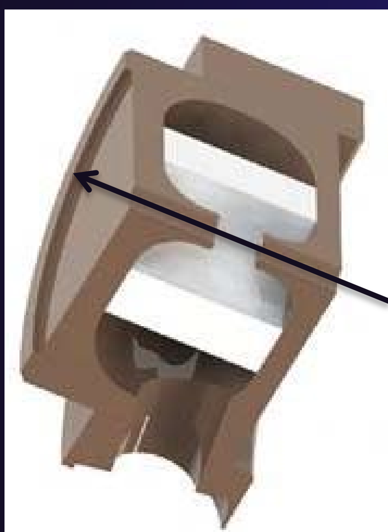
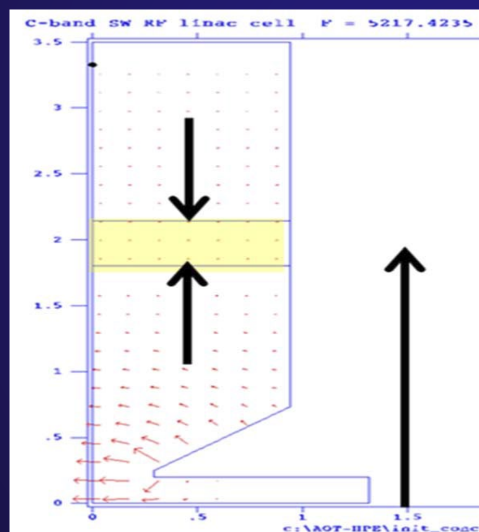
  - Integrate NCRF-design concepts with cryogenic operation
- Prior R&D efforts
  - **Exploit integration of dielectrics for increased SWaP of accelerator in Space (AIS) systems**

# Performance improvements by introduction of dielectrics

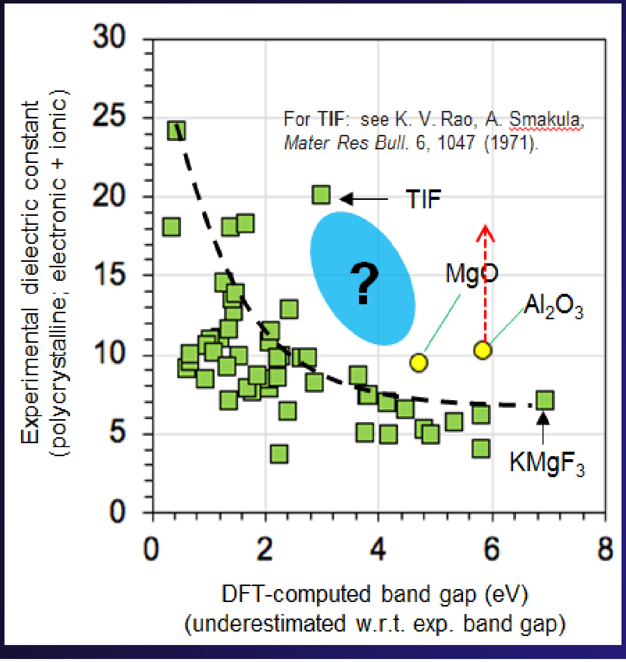
- Configuration that reduces potential charge-up
- Design leads to improved efficiency and reduced size



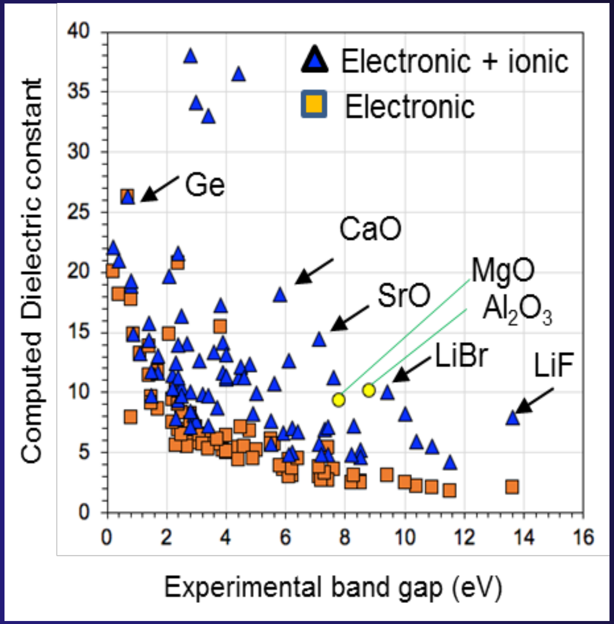



| Epsilon | $R_{cav}$ | Ceramic Width | Ceramic R frac | $P_{cav}$ |
|---|---|---|---|---|
| | [cm] | [cm] | [cm] | [W] |
| 1 | 4.64 | N/A | N/A | 134 |
| 3 | 4.00 | 0.65 | 0.59 | 89.5 |
| 5 | 3.80 | 0.544 | 0.56 | 78 |
| 6 | 3.78 | 0.494 | 0.56 | 76 |
| 8 | 3.65 | 0.426 | 0.56 | 72 |
| 10 | 3.62 | 0.360 | 0.54 | 70 |
| 15 | 3.56 | 0.312 | 0.56 | 66 |
| 20 | 3.59 | 0.268 | 0.52 | 64 |
| 20 | (addit'l geometry optimization) | | | 60 |

# Theoretical study of dielectrics for new options or custom design




Dielectric constant versus bandgap (computed within DFT) plot for a set of polycrystalline ceramic materials previously reported in literature. Yellow circles identify materials that have been proposed as promising dielectrics for the hybrid cryogenic copper/ceramic accelerator. The arrow at the alumina dot shows the doping Euclidlabs did for our test dielectric.




Dielectric constant versus experimental bandgap plot for all binary octet AB-type compounds. Yellow circles identify materials that have been proposed as promising dielectrics for the hybrid cryogenic accelerator and other compounds with comparable performance are highlighted.

- High dielectric constant and large bandgap (low losses) are desirable
- Most materials have one or the other
- Can new materials be designs (like Ti-doped alumina)?
- Do compromise materials have good vacuum and/or breakdown properties?

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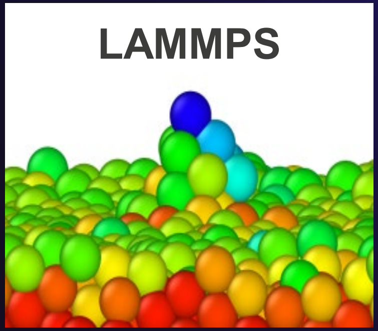
  - Integrate NCRF-design concepts with cryogenic operation
- Prior R&D efforts
  - Exploit integration of dielectrics for increased SWaP of accelerator in Space (AIS) systems
- **Building a ollaboration with other US efforts for full accelerator system**
  - **TOPGUN photo-injector development at UCLA (Rosenzweig)**
  - **RF-structure and coupler technology at SLAC (Tantawi)**
  - **RF-power systems for operation of UHG structures  at SLAC (Kemp)**

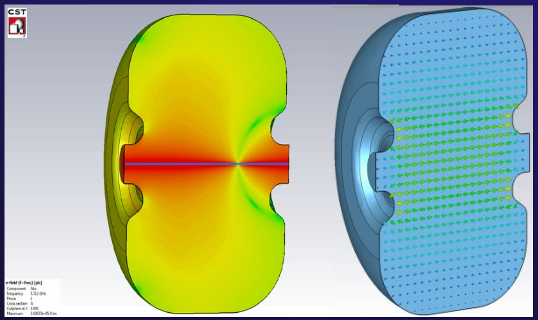
# Full Technology R&D efforts

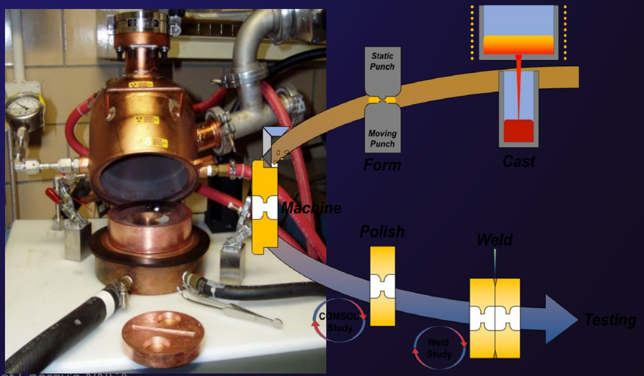
Proposal for a full 3-year effort related to high gradient operation

- Develop theoretical understanding of breakdown and its precursors
- Develop recipe for best materials to build UHG RF-structure
- Design resonator and coupler configuration for UHG RF-structure
- Develop metallurgic and fabrication concepts to build these
- Integrate design and fabrication with best cryogenic configuration
- Perform sample testing experiments
- Build and RF-test UHG prototypes
- Build extendable test stand with source, high-power klystron and RF-structure to beam-test of UHG structure

**Material Science + RF Engineering + Advanced manufacturing**



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**Proposal for a full 3-year effort related to the use of dielectrics**

- **Continue study of suitable dielectrics (low loss, suitable for high fields)**
- **Design, build and test RF-structures with integrated dielectrics**

# Summary and Outlook

- LANL is in the process of starting a up to 4 year program for an integrated UHG resonator development that includes
  - material simulations to understand and improve breakdown behavior
  - C-band has been identified as the most suitable frequency for LANL needs
  - Establish standing-wave RF-structure designs for long-pulse operation
  - Use LANL advanced manufacturing capabilities for “gentle” manufacturing
  - Start up a electron beam testing capability (ADEF). Beamline is expected to be extended by other programmatic needs. Test bed for diagnostics, RF-structure, and cathode development, including small FEL experiments.
  - Establish dielectric for performance improvement at moderate gradients
- The developed technologies are expected to
  - Establish custom material designs for high performance RF resonators
  - Provide the foundation for an improved LANL-XFEL design
  - Provide technologies for compact FEL designs
  - Establish a path to transportable SNM detection devices using ICS gammas

# Acknowledgements


Contributions from:

- Evgenya Simakov, John Lewellen, Mark Kirshner, Ari Le, Tim Germann, Danny Perez, Gaoxue Wang, Ghanshyam Pilania, Andrew Garmon, Samantha Lawrence, Amber Black, and Todd Jankowski at LANL
- Sami Tantawi and Emilio Nanni at SLAC
- Jamie Rosenzweig and Atsushi Fukasawa at UCLA


THE END

# High Gradient Collaboration

- FY19 Work
  - LANL effort to secure the 3-year funding for both C-band and dielectric work
  - Establish MOU between SLAC, UCLA and LANL on collaboration
  - Dielectric characterization of Ti-doped alumina at SLAC
  - Detailed quantification of S- vs. C- vs X-band performance of RF-resonators
  - Cost comparison for full 12 GeV linac
  - Design of S-band tank with distributed coupling w/ optimization of short-range wakes
  - Fabrication of prototype with testing at UCLA by the end of the year
  - Participate in cFEL activities led by UCLA & SLAC
    - Share material simulation results
    - Share design of S-band proof-of-principle resonator (scaled from wake-optimized C-band design)
    - Share expertise on eSASE concepts

# High Gradient Collaboration

- FY20-22 Work (SLAC and UCLA will partner with LANL)
  - Establish better copper or copper alloy for breakdown suppression, or at a minimum provide molecular dynamics based explanation for the experimental findings
  - Design and build a prototype C-band structure at LANL
  - Aquire a C-band, high peak-power klystron
  - Set up a simple beamline for a beam-tests at C-band (ADEF)
  - Contribute to trade-off study on ILC type accelerator with SLAC
    - Share C-band optimization results
    - Trade-off between fewer high-power tubes and many lower power tubes